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Title: Influence of twin-grain boundary interactions on further twin growth and twin transmission in HCP metals

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INFLUENCE OF TWIN GRAIN BOUNDARY INTERACTIONS ON FURTHER TWIN GROWTH AND TWIN TRANSMISSION IN HCP METALS

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"Multiscale Study of the Role of Microstructure in the Deformation Behavior of HCP Materials"

BES-DOE Project FWP 06SCPE401

Collaborators: M. Arul Kumar, I.J. Beyerlein*

* Mechanical Engineering & Materials Dept, UC Santa Barbara, USA

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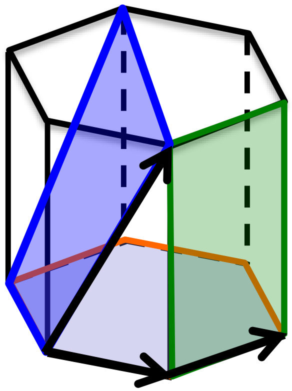
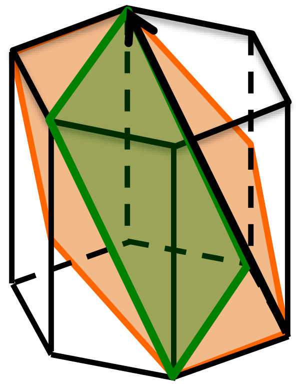
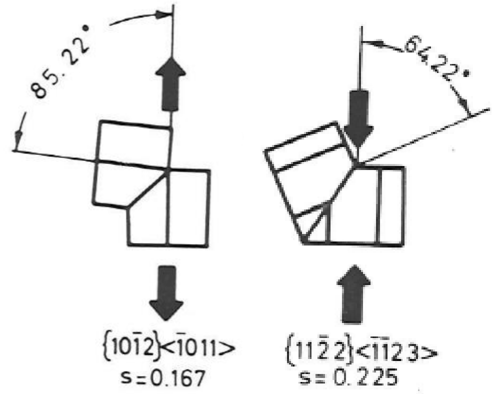
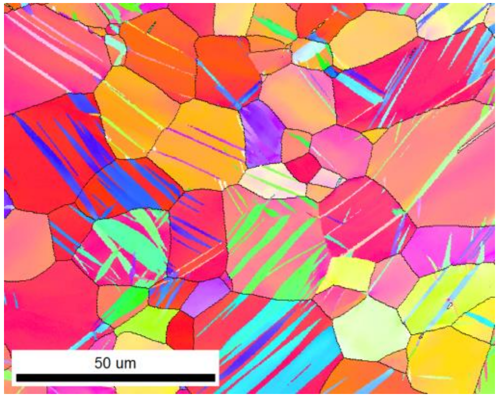
Plasticity of hexagonal materials

Several slip and twin modes with different activation threshold and high anisotropy







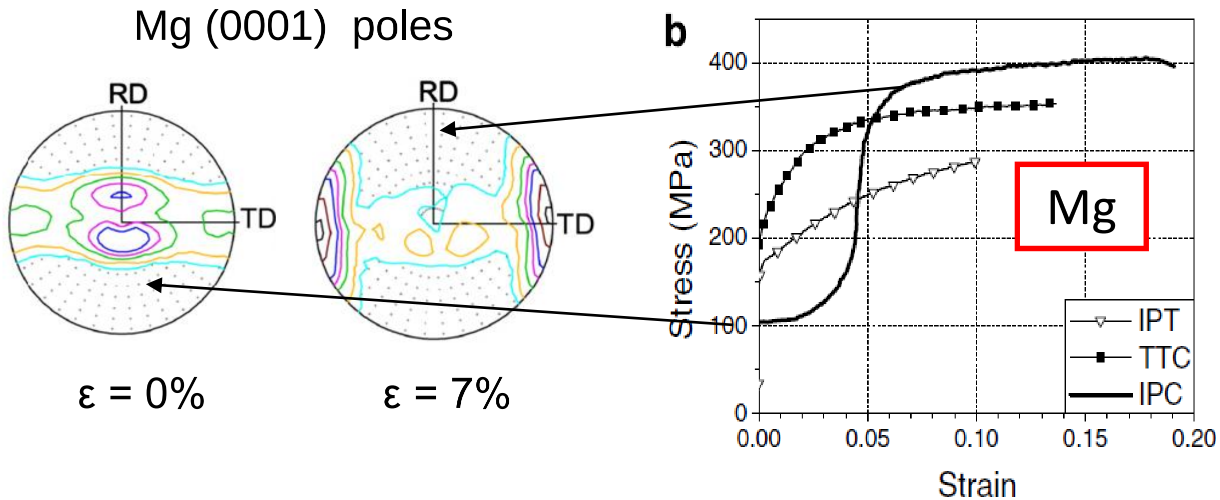


<a> slip: prism, basal
<c+a> slip: pyramidal

(10-12) tensile twin
(11-21) tensile twin

Twinning and phase transformation affects texture, hardening, anisotropy, ductility

Mg (0001) poles



Proust et al., IJP (2009)

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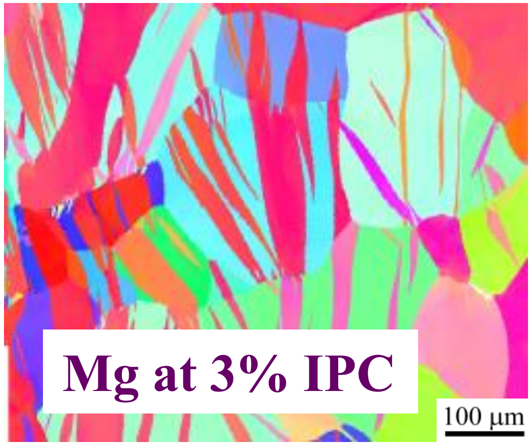
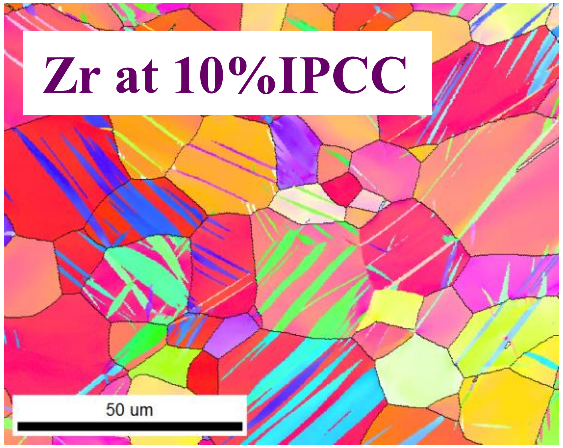
Deformation twins in HCP metals

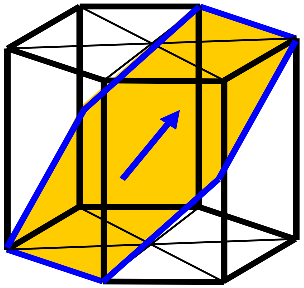
Twin transmission across grain boundaries (Adjoining Twin Pairs)



(Beyerlein et al., Phil Mag, 2010)



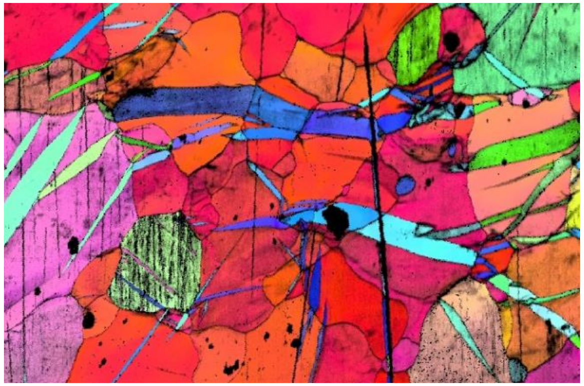
(Capolungo et al, Acta Mat, 2009)



Twin type : Tensile twin $\{10\bar{1}2\}$

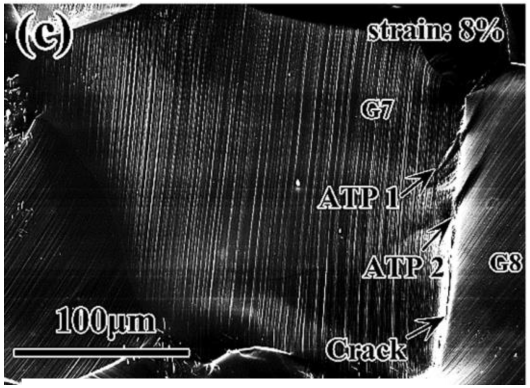
Adjoining twin pairs, twin chains and fracture in HCP metals

Twin chain in Mg



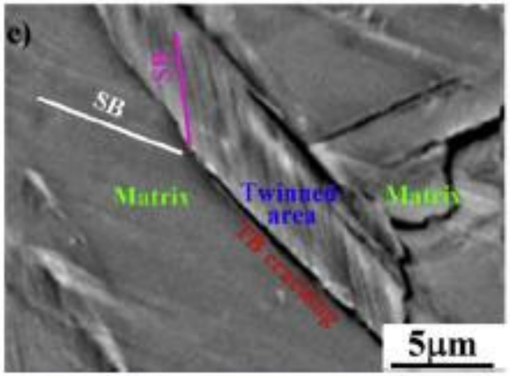
(Arul Kumar et al., Under prep)

Crack nucleation at ATPs



H. Yue et al., MSE-A, 2016)

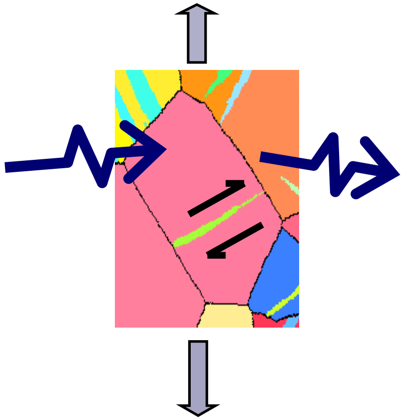
Twin boundary cracking

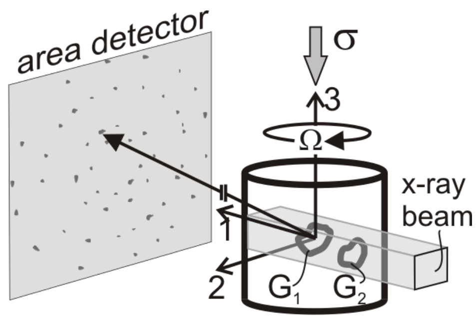


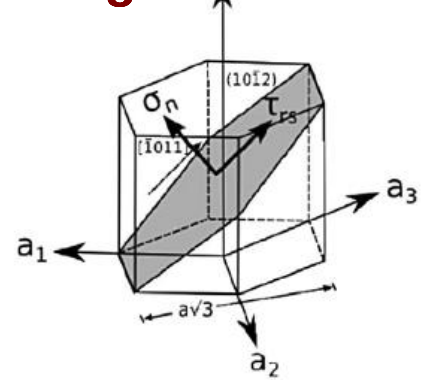
Twin chains may enhance twin boundary cracking and premature fracture

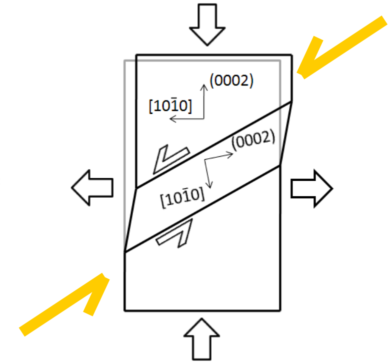
Internal stresses associated with twinning: measurements

X-ray synchrotron measurement of average stresses in the twin and in the parent grain in Mg AZ31

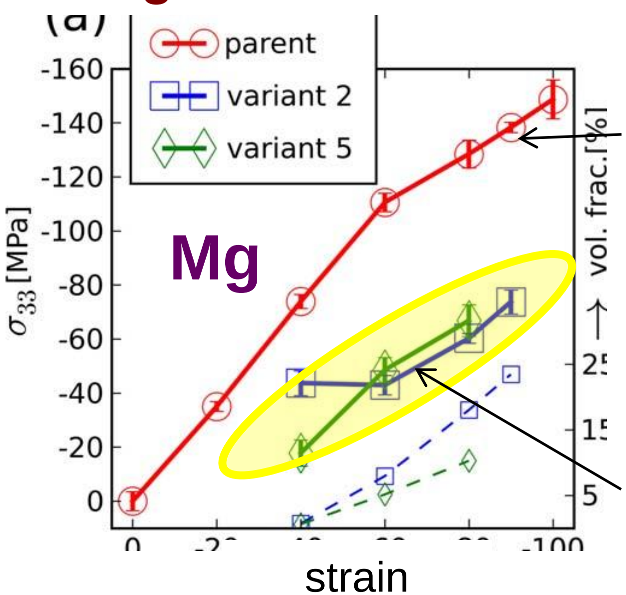






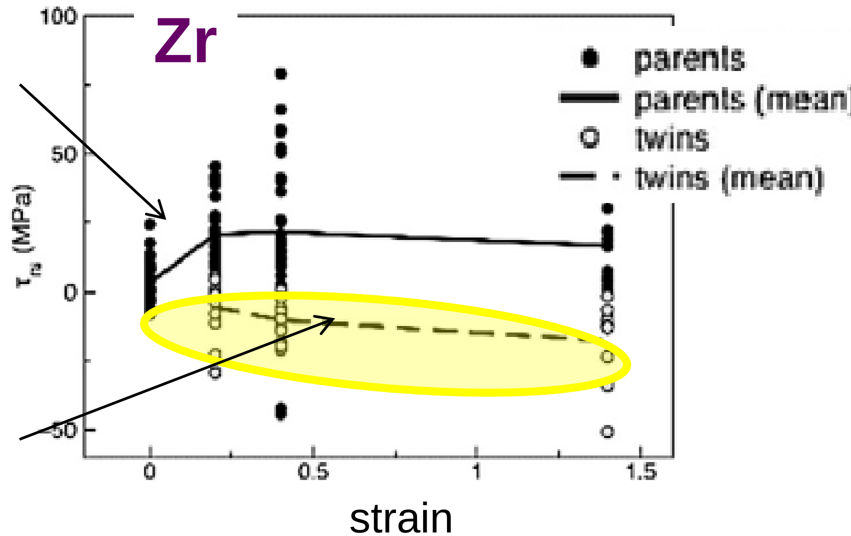


Average resolved shear on twin plane (10-12) for parent and twin



RSS in parent

RSS in twins



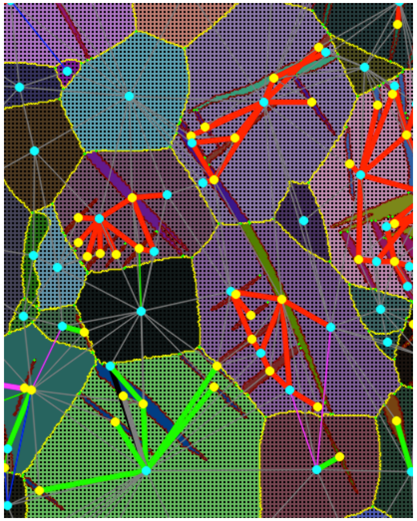
Aydiner et al., PRB 80 (2009) 024113

Abdolvand et al., IJP 70 (2015) 77-97

Experimental and Numerical Tools

Automated EBSD statistics

→ used to identify relevant mechanisms and to establish correlations

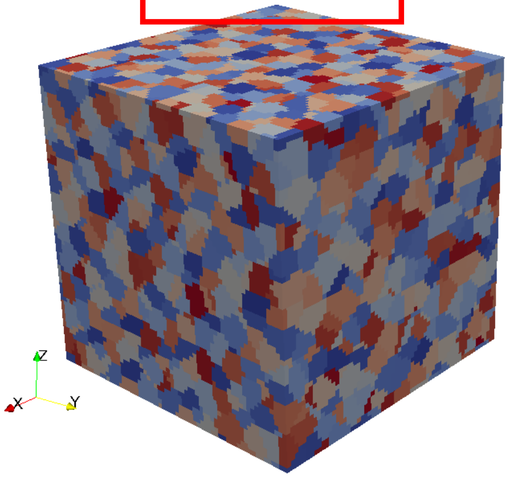


- Marshall et al, J. Microscopy 238 (2010) 218
- Juan et al., Acta Mater (2015)

Elasto-Visco-Plastic Fast Fourier Transform

$$\boxed{\sigma_{ij,j} = 0}$$

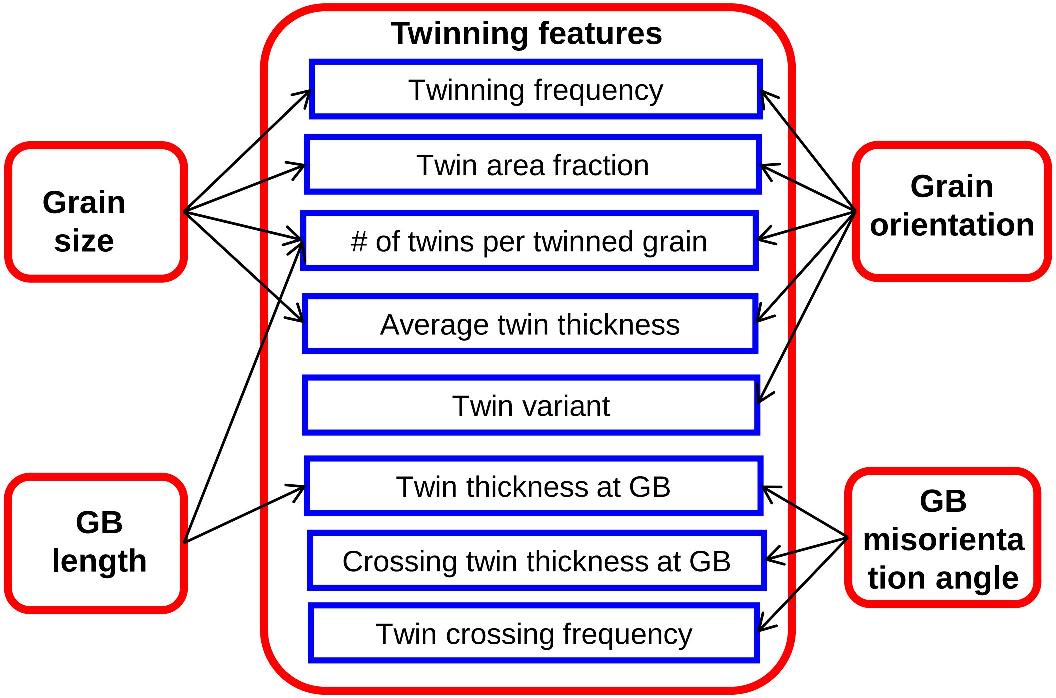
→ a spatially resolved crystal plasticity approach used to solve equilibrium equation and calculate local stresses in aggregate



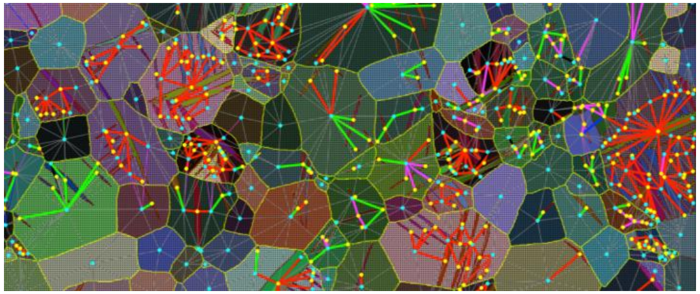
* Lebensohn, Acta Metall **49** (2001) 2723-37
* Lebensohn, Kanjarla, Eisenlohr, IJP **32-33** (2012) 59-69

Statistical characterization of twins by EBSD

Statistics are performed using automated EBSD software to characterize micro structure, with an emphasis on twinning features



Processing EBSD image



DATABASE (in SQL basis)

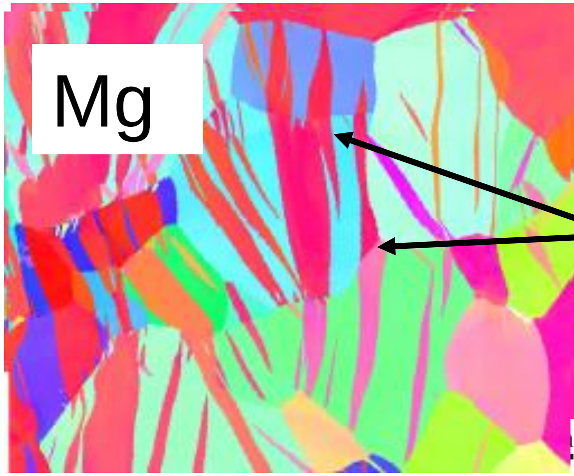
DATA PROCESSING
(automated using shell scripts, SQL requests, fortran/C++ programs and gnuplot)

	Mg	Zr	Ti
# of grains	2339	1200	4678
# twinned grains	1534	530	1386
# of twins	8550	1975	2331

- Zr EBSD analysis: Juan et al., Acta Mater (2015)
- Mg EBSD analysis: Beyerlein et al, Phil. Mag (2010); Arul Kumar et al (under preparation)
- Ti EBSD analysis: Wronski et al (under preparation)

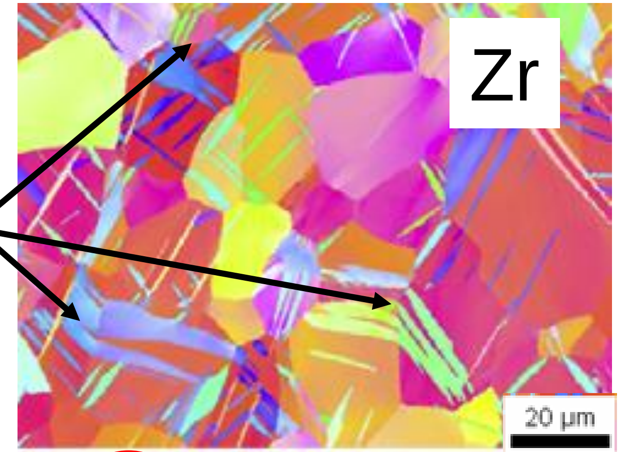
Twin transmission across grain boundaries

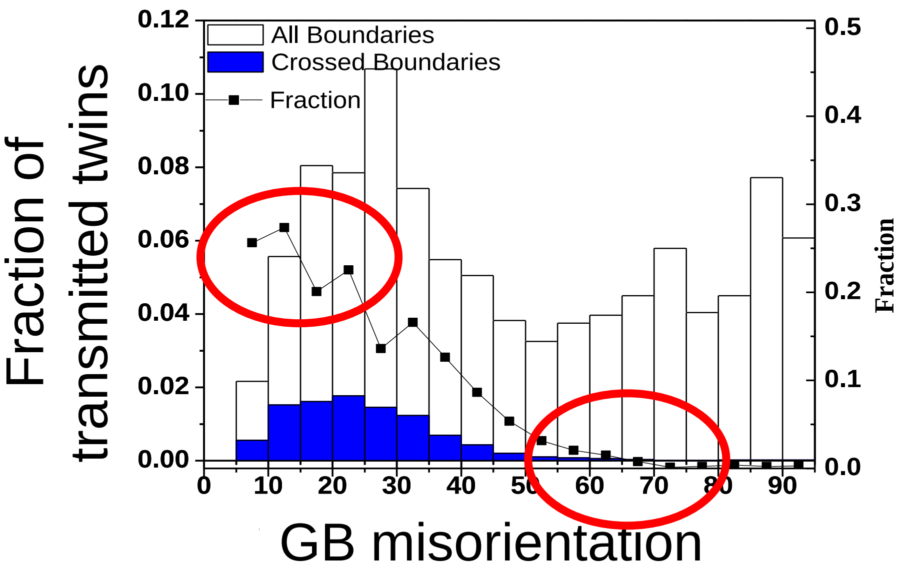
Magnesium at 3% IPC

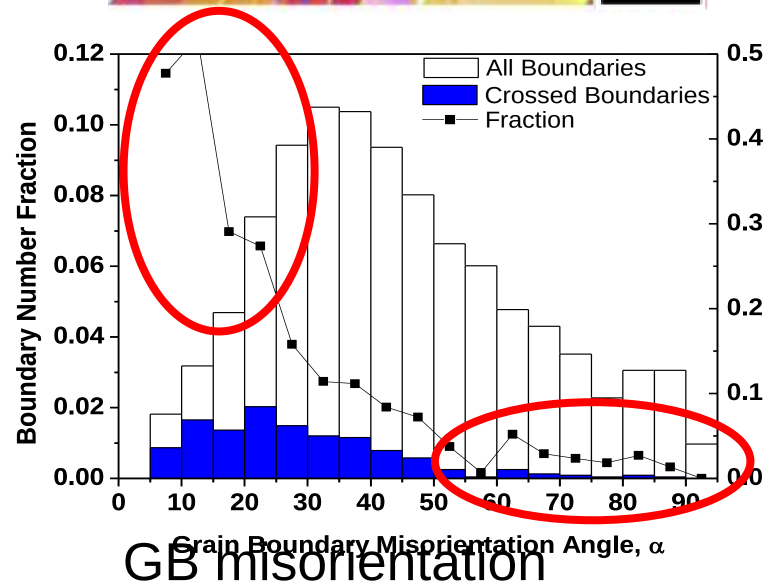


Twin pairs joined at grain boundaries

Zirconium at 10%IPC

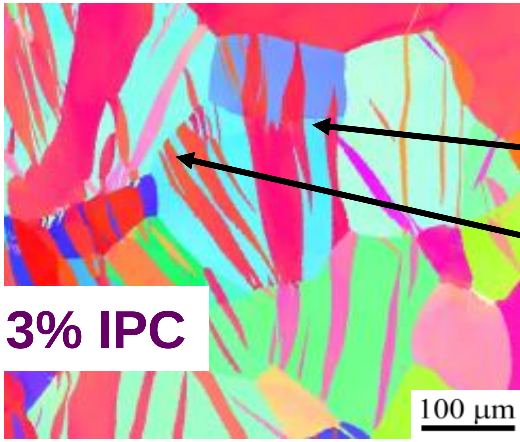






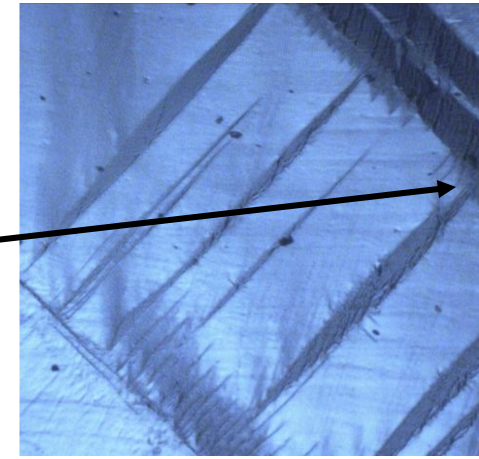
Adjoining twin pairs (ATP) are observed at low misorientation boundaries

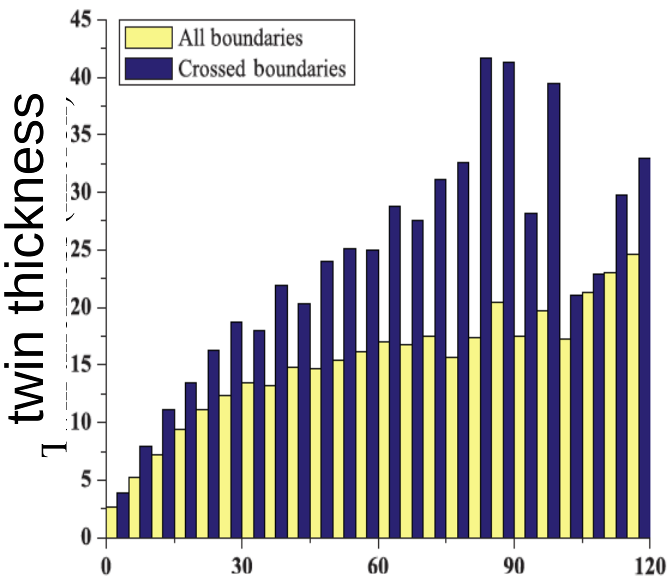
Crossing twin thickness at grain boundary



Crossing twin at grain boundary

Non-crossing twin at grain boundary



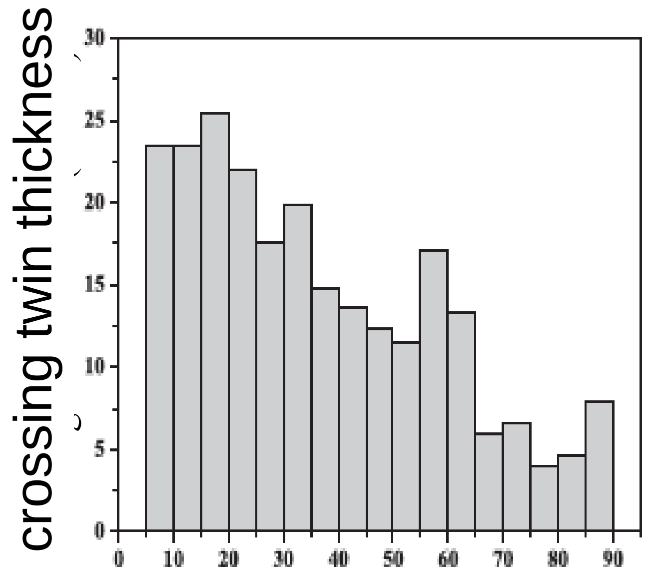


Grain bound length

Crossing twin thickness at GB:

High compared to non-crossing twin thickness at GB

Decreases with increasing misorientation



Grain bound misorient

Situations where experiments cannot accurately characterize stress

- Effect of neighboring grain on twin local stresses
- Effect of twin-induced stresses on:
  - Twin transmission across grain boundaries
  - Crossing twin thickness
  - Twin growth

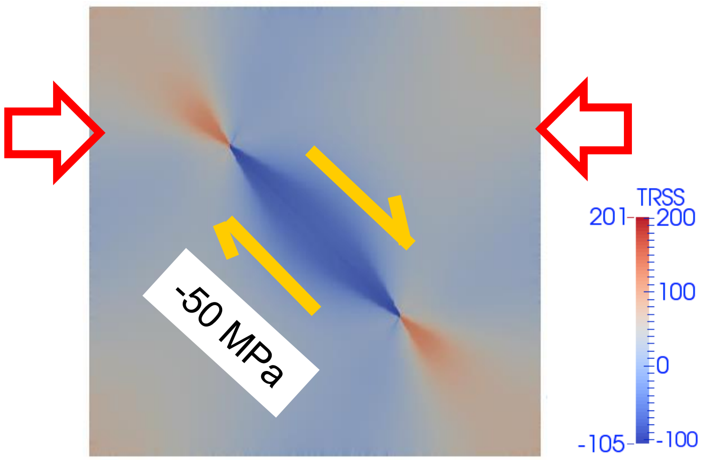
STRATEGY: Solve equilibrium equation and calculate local stresses associated with twins using a Fast Fourier Transform method and a crystal plasticity constitutive law

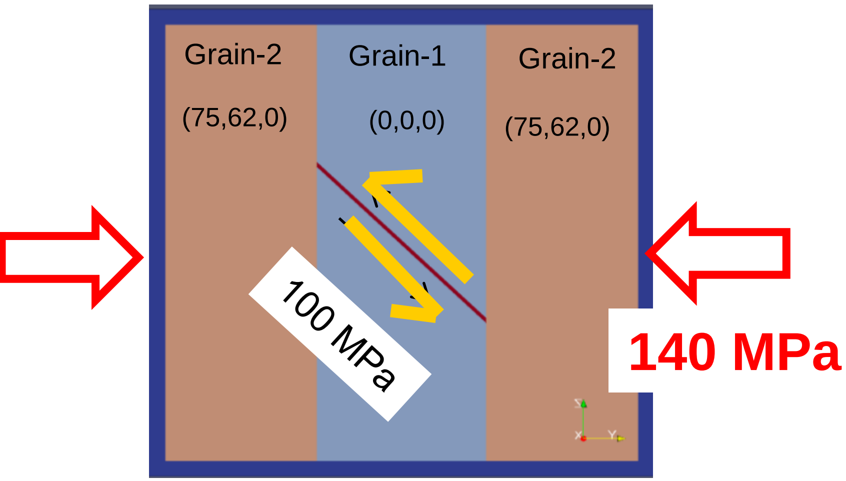
M. Arul Kumar, A.K. Kanjarla, S.R. Niezgoda, R.A. Lebensohn, C.N. Tomé, "Numerical study of the stress state of a deformation twin in Mg", Acta Materialia 84 (2015) 349-358

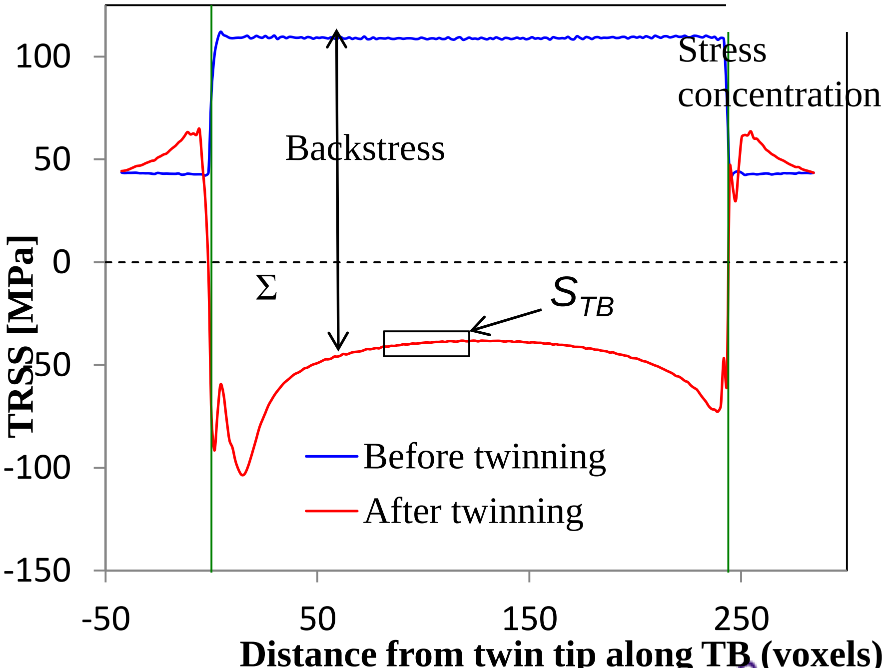
FFT based twin local stresses (Zr case)

- Twin transformation induced by macroscopic compression (140 MPa) of a grain included between two grains
- Basal/prism/pyramidal/twin → 200 /20 /160/100 MPa
- Twin transformation is enforced as a 13% shear imposed via 2000 small increments under a constant stress of 140 MPa

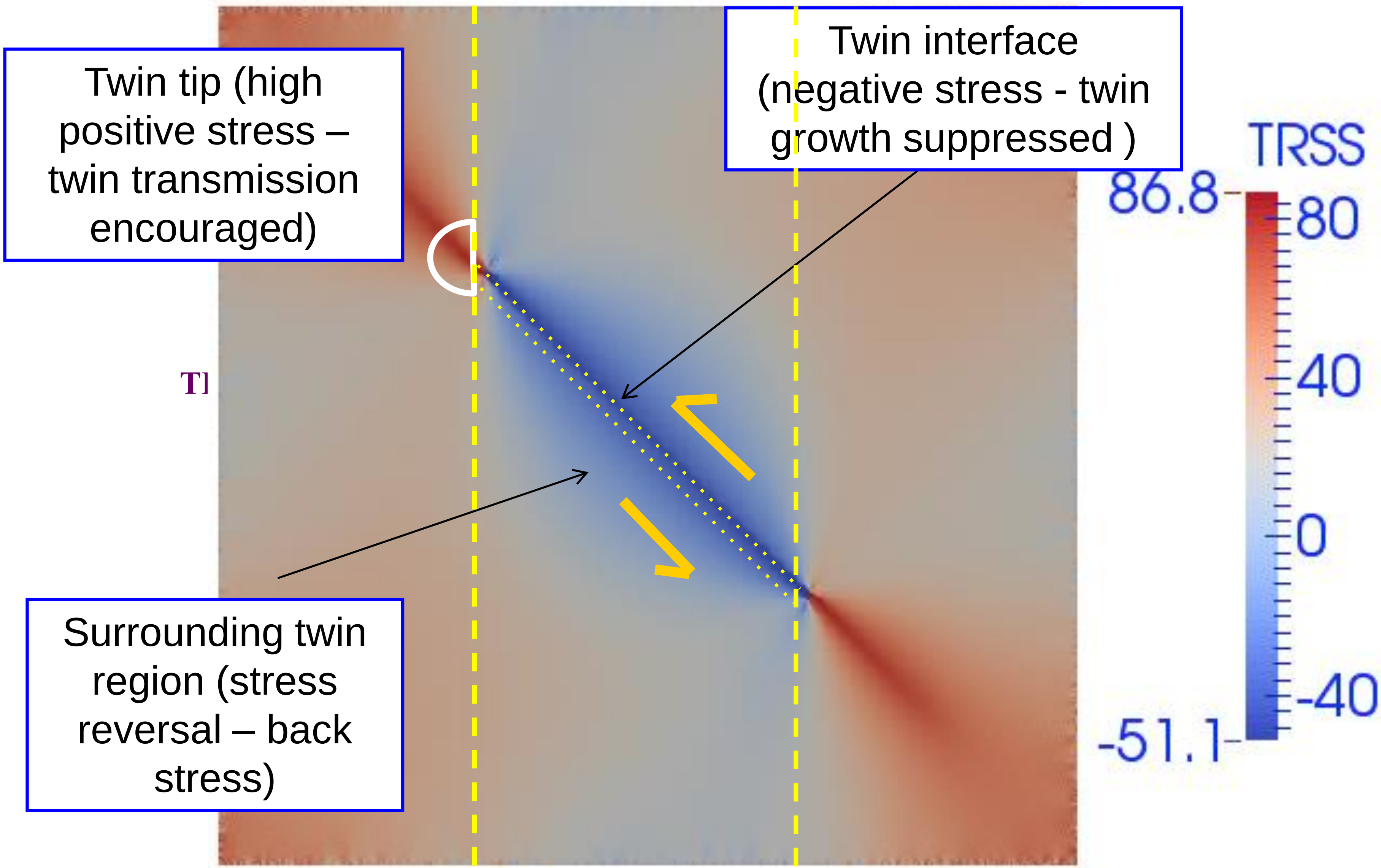
Resolved shear on twin plane







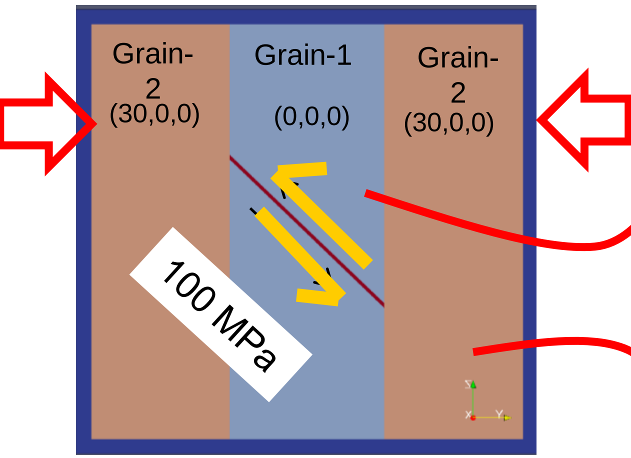
Twin-plane Resolved Shear Stress (T-RSS) distribution

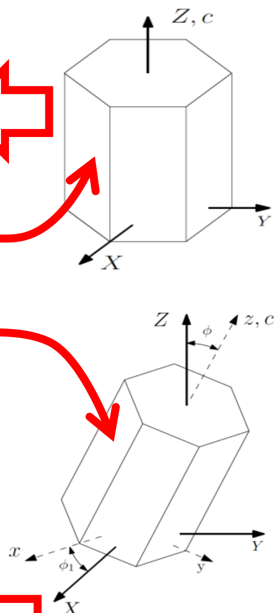


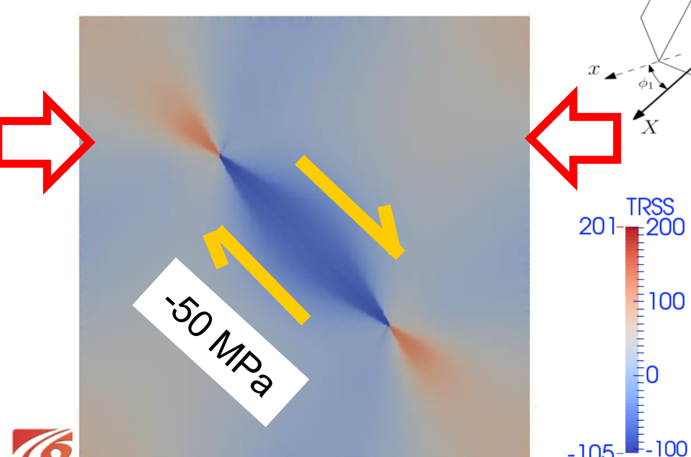
Accommodation of twinning shear transformation induces local plasticity and strong stress heterogeneity

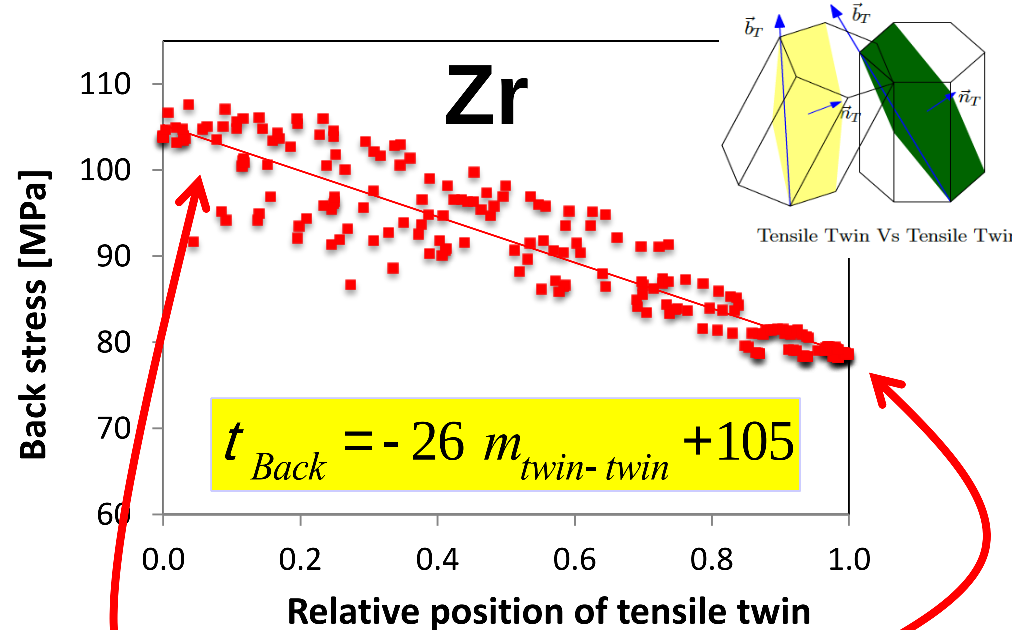
Zr: effect of neighboring grain crystallography on back stress

FFT simulation of twin transformation with different neighboring grains
→ the back stress depends on how much plastic accommodation takes place in the neighbor









tensile twin in neighbor not well aligned with parent twin

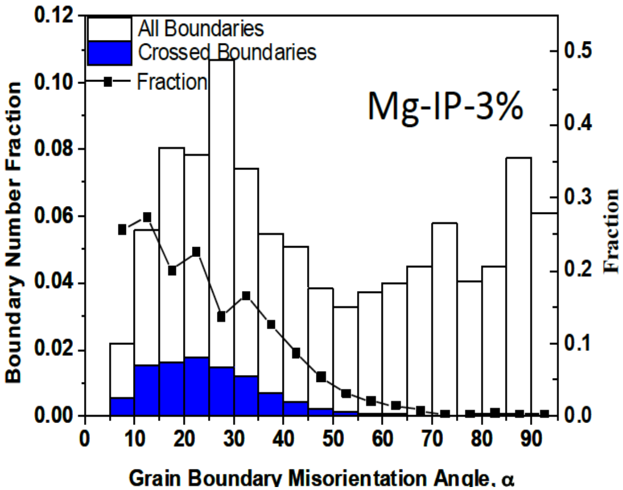
tensile twin in neighbor well aligned with parent twin

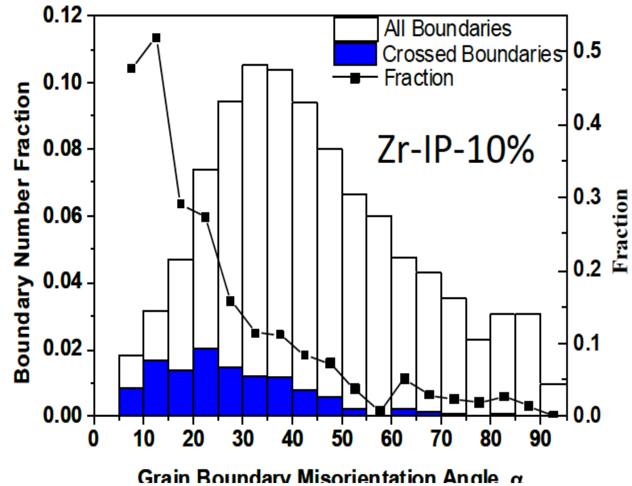
Situations where experiments cannot accurately characterize stress

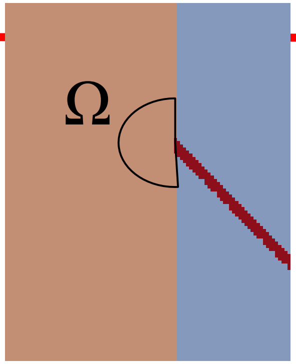
- Effect of neighboring grain on twin local stresses
- Effect of twin-induced stresses on:
  - ➢ Twin transmission across grain boundaries
  - ➢ Twin growth
  - ➢ Twin separation

M. Arul Kumar, I.J. Beyerlein, R.J. McCabe, C.N. Tomé, “Grain neighbor effects on twin transmission in HCP materials”, Nature Communications 7:13826 DOI: 10.1038/ncomms13826 (2016)

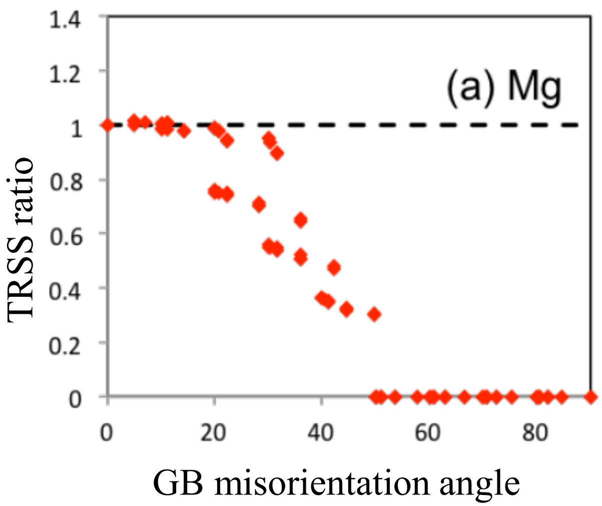
Twin transmission across grain boundary

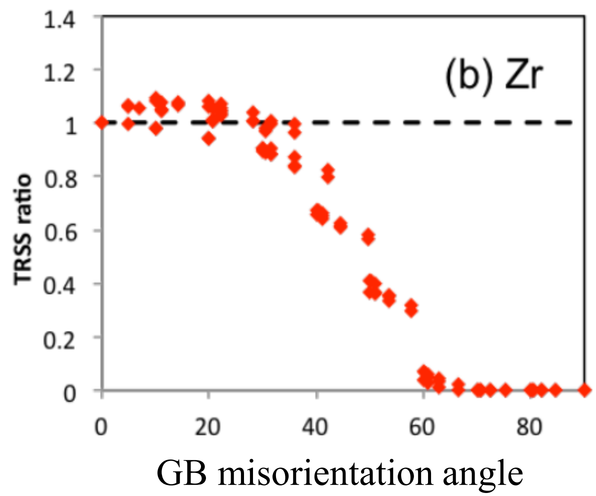


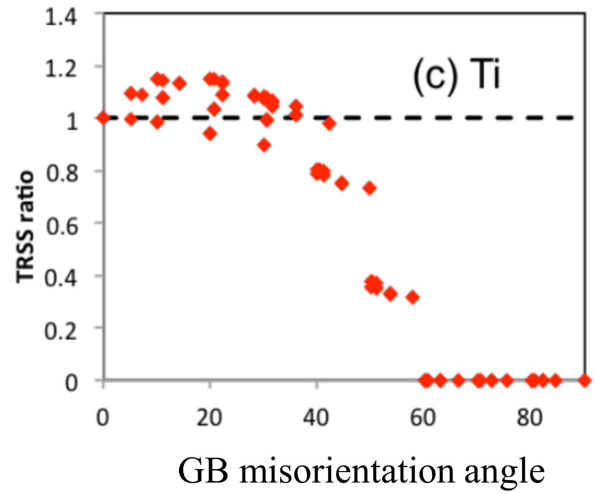




$$t^{RSS}_{ratio} = \frac{t^{RSS}_{max}\big|_{W}}{t^{RSS}_{max}\big|^{SX}_{W}}$$

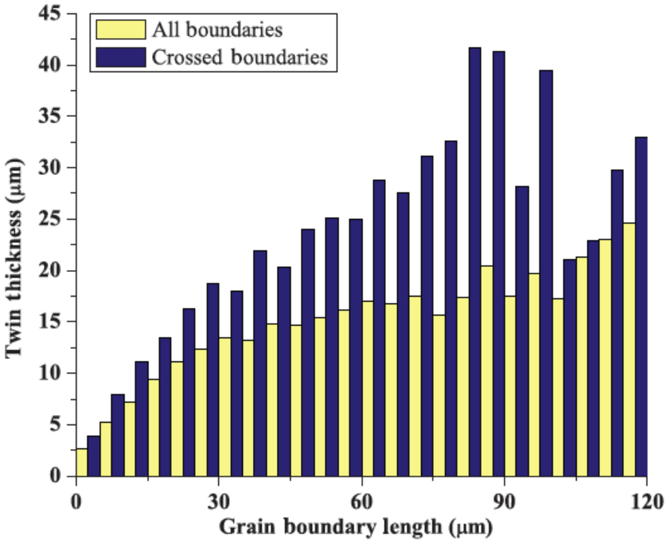


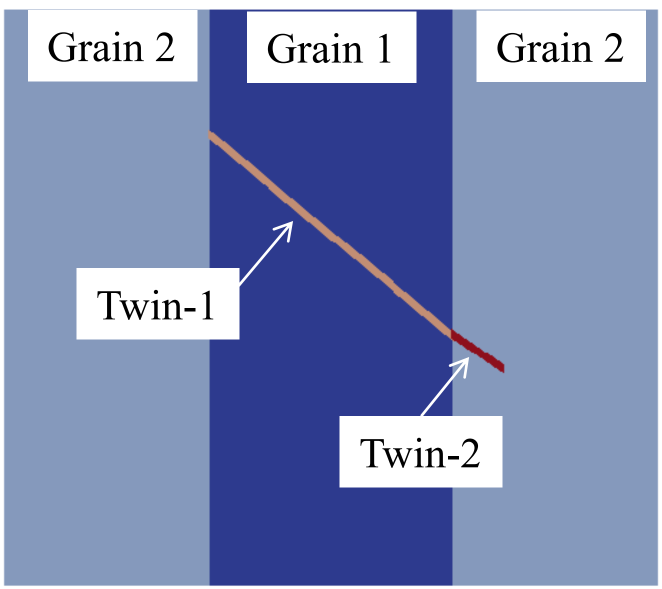




Adjoining twin pairs are preferred at low misorientation boundaries; and more likely in relatively high anisotropic Zr than in Mg

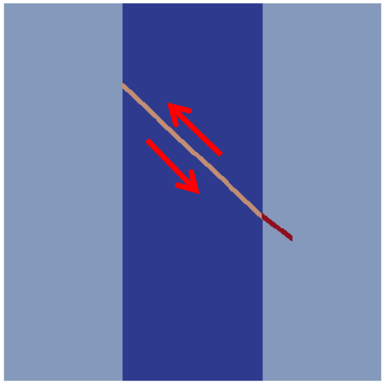
Crossing twin thickness at grain boundary : FFT simulation



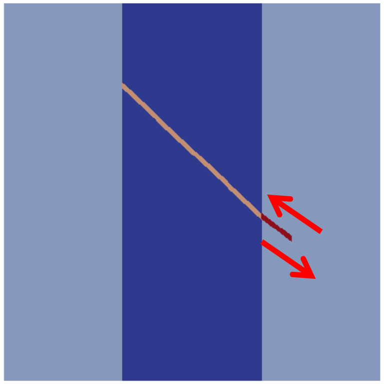


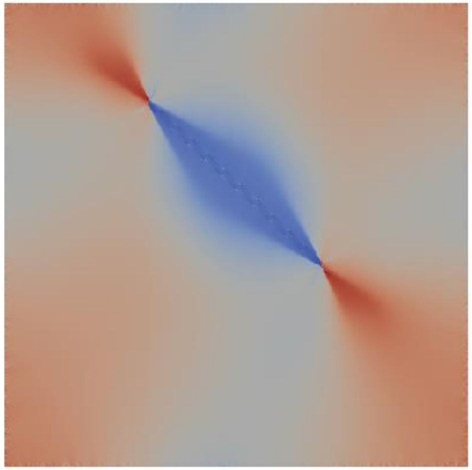
Mis-orientation at GB: θ= 5°

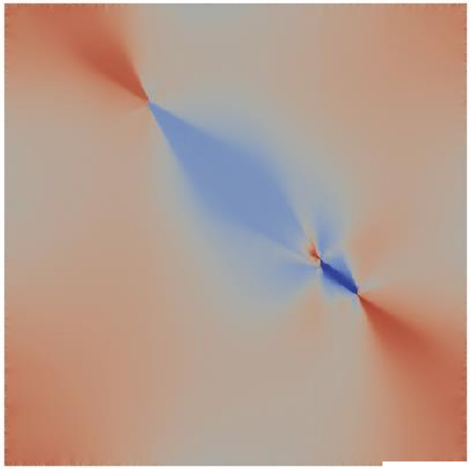
Shear Trans. of twin 1

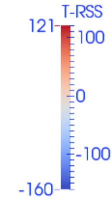


Shear Trans. of twin 2



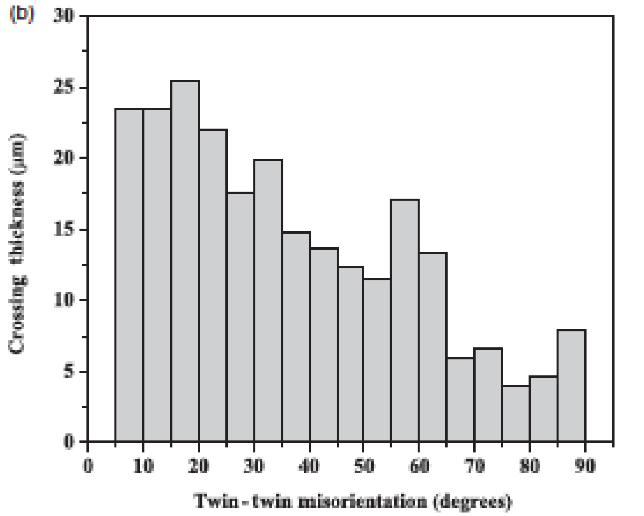


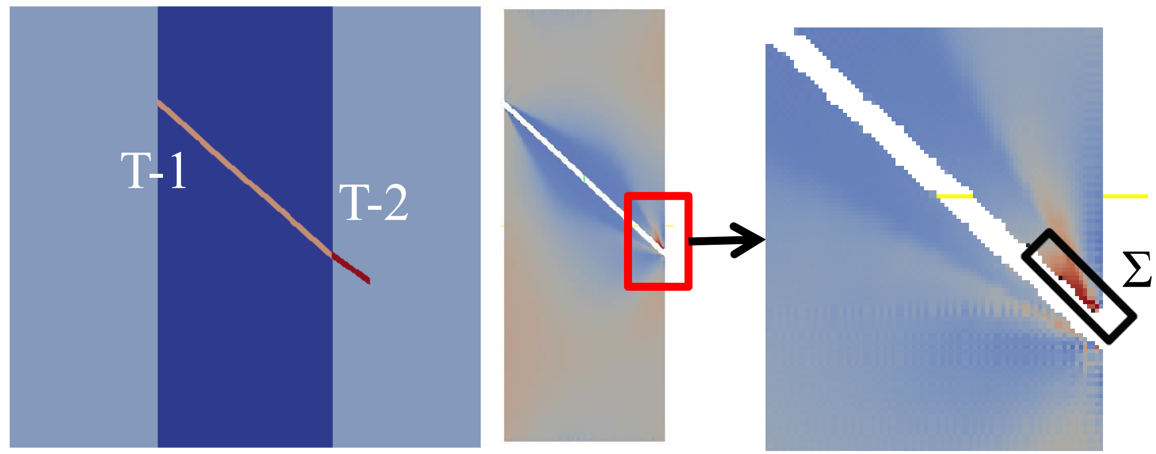




Twinning shear transformation of T-2 relaxes the back stress associated with T-1

grain boundary misorientation and crossing twin thickness



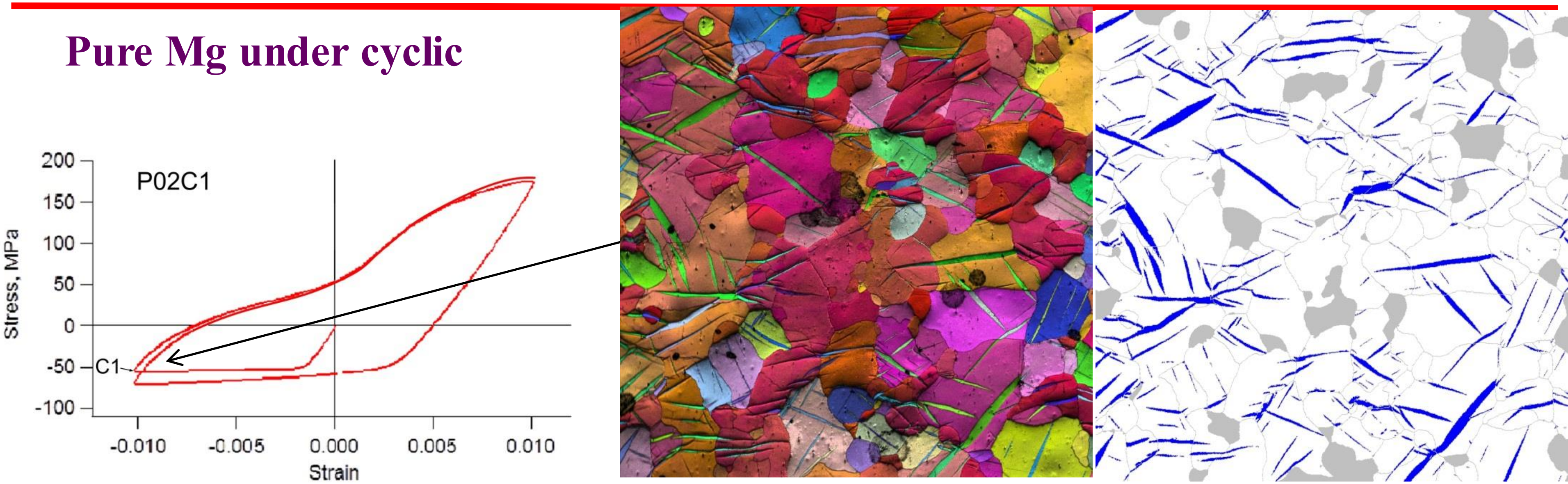


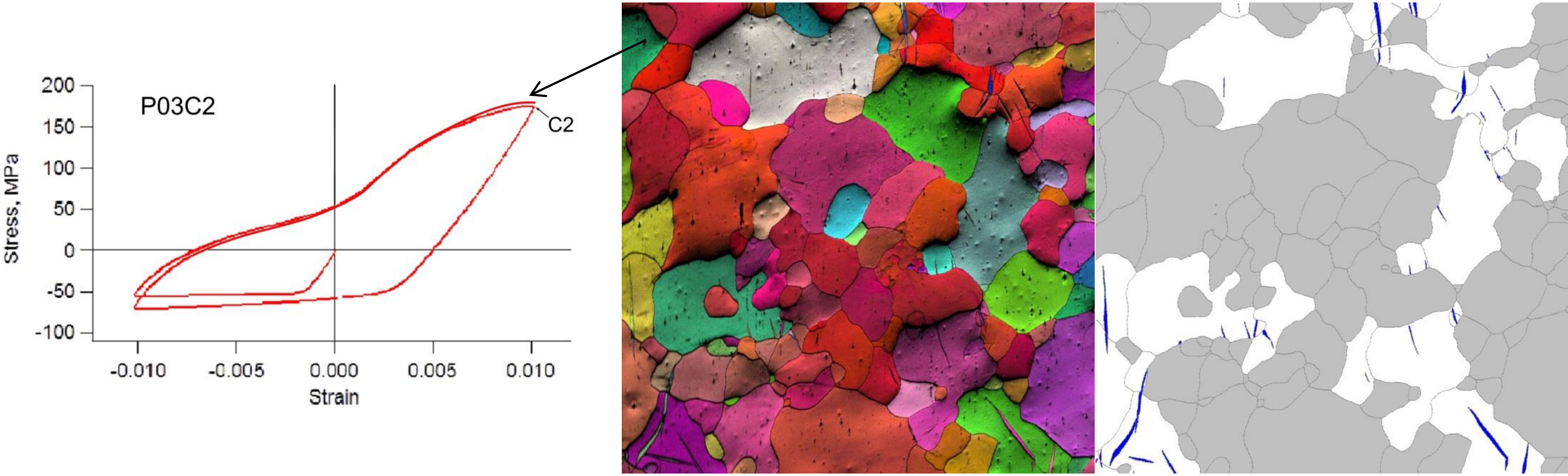
Misorient angle at GB	T-RSS in region Σ			
	Mg		Zr	
	Twin-1 transf	Twin-2 transf	Twin-1 transf	Twin-2 transf
10°	-49 →	29	-85 →	93
20°	-41 →	17	-86 →	79
30°	-37 →	-34	-89 →	49

Local back stress is relaxed when Twin 2 is formed, which helps growth and so increase twin thickness at grain boundary

Twinning behavior under cyclic loading (preliminary results)

Pure Mg under cyclic





Detwinning of ATPs under load reversals is less favorable compared to isolated twins due to local back stress relaxation at GB of ATPs

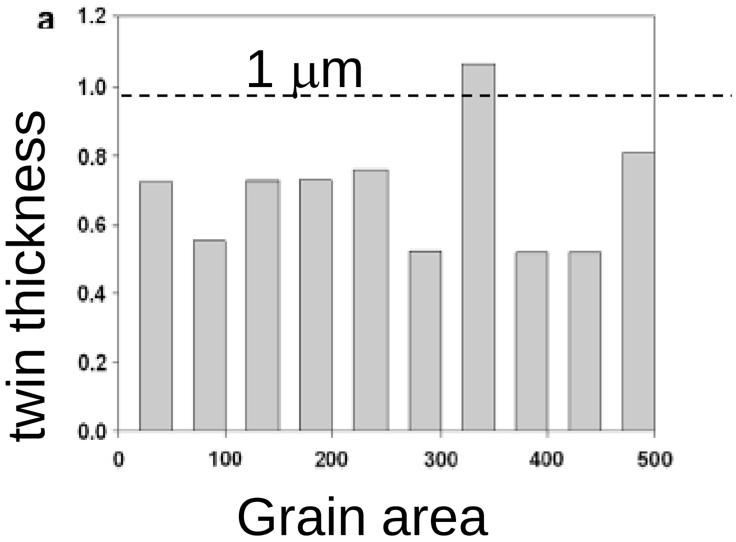
Situations where experiments cannot accurately characterize stress

- Effect of neighboring grain on twin local stresses
- Effect of twin-induced stresses on:
    - Twin transmission across grain boundaries
    - Twin growth
    - Twin separation

M. Arul Kumar, I.J. Beyerlein, C.N. Tomé
"Effect of local stress fields on twin characteristics in HCP metals"
Acta Materialia 116 (2016) 143-154

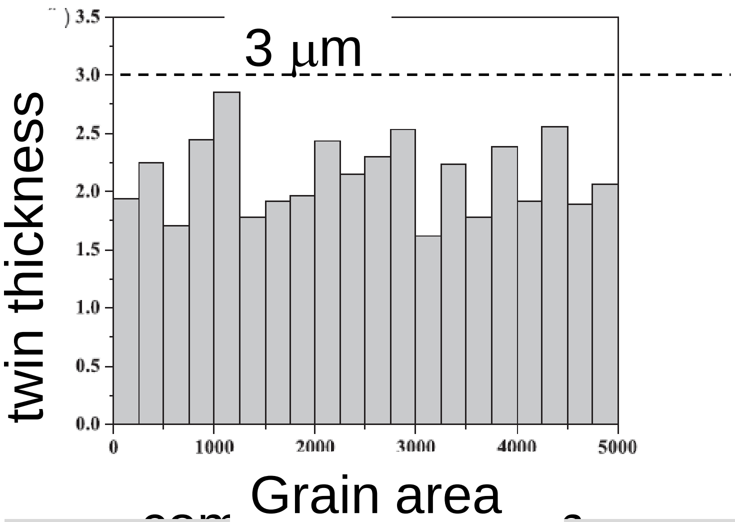
Effect of twin local stresses on twin growth

Zr



Capolungo et al, Acta Mat (2009)

Mg

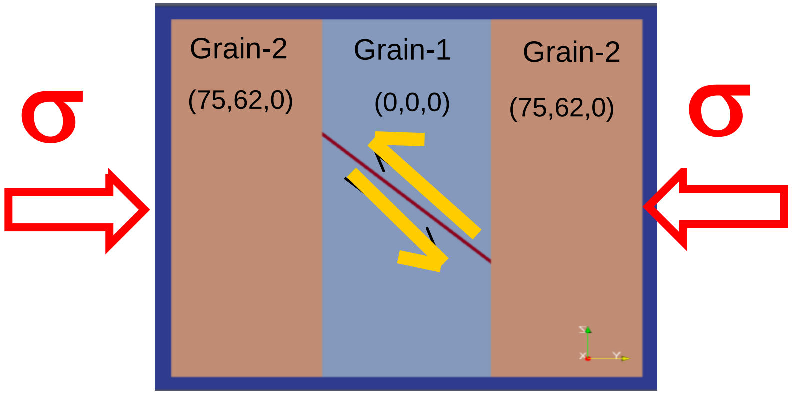


Beyerlein et al, Phil Mag (2010)

Automated EBSD shows that twins are (in average) thinner in Zr than in Mg, independently of grain size

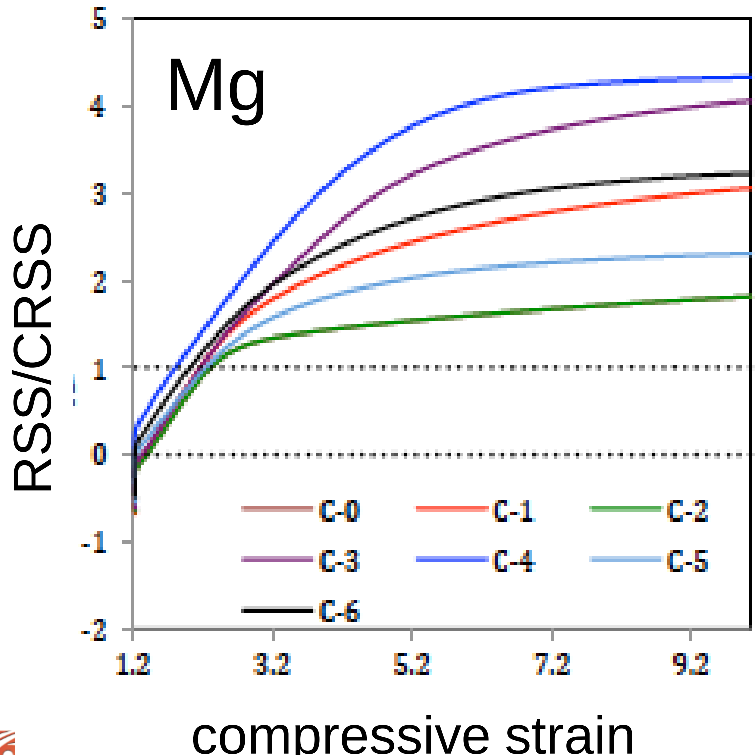
We show below that increasing the applied stress reverses the back stress on the twin by different amounts in Zr and Mg

Effect of twin local stresses on twin growth



Apply increasing compressive stress on system and follow evolution of RSS on twin

When RSS/CRSS>1 twin will grow



Do for different neighbors

Mg

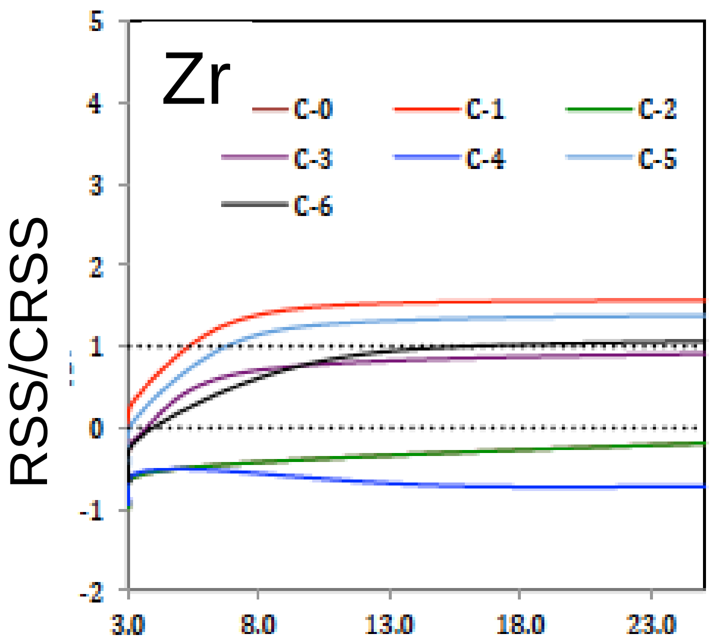
→ lower plastic anisotropy

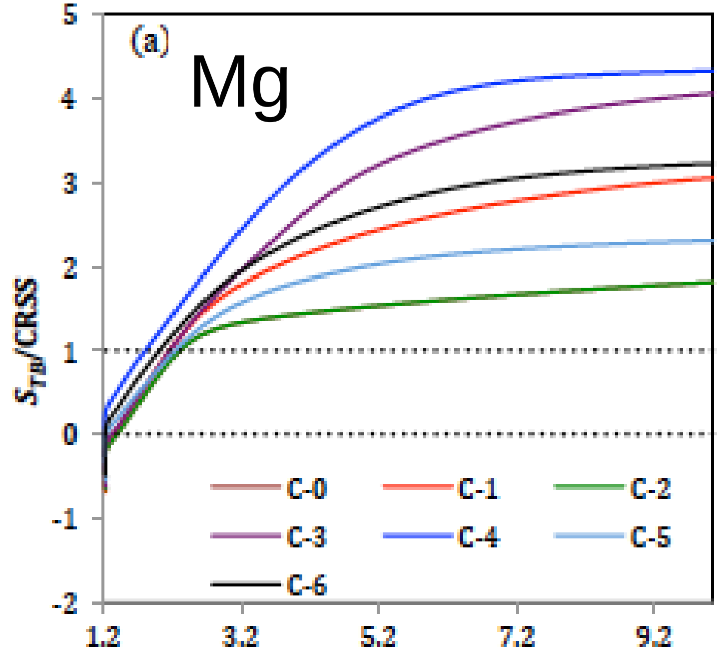
→ higher forward shear accommodation in neighbor

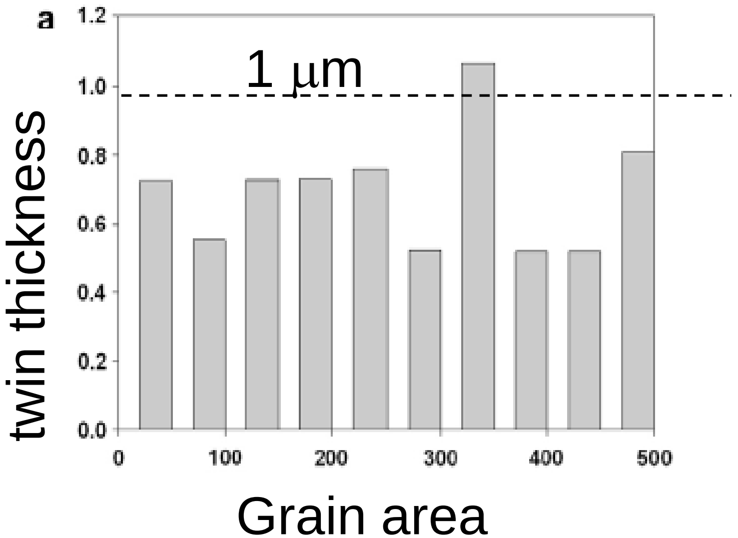
→ lower back stress on twin

→ more twin growth

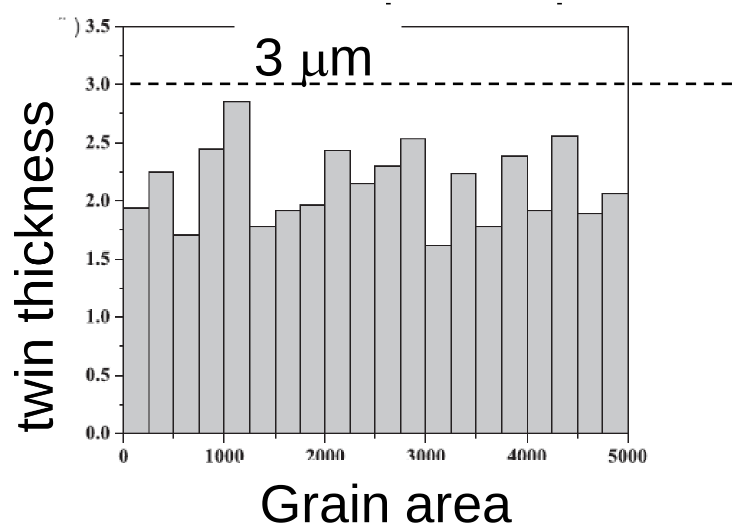
Effect of twin local stresses on twin growth







Capolungo et al, Acta Mat (2009)



Beyerlein et al, Phil Mag (2010)

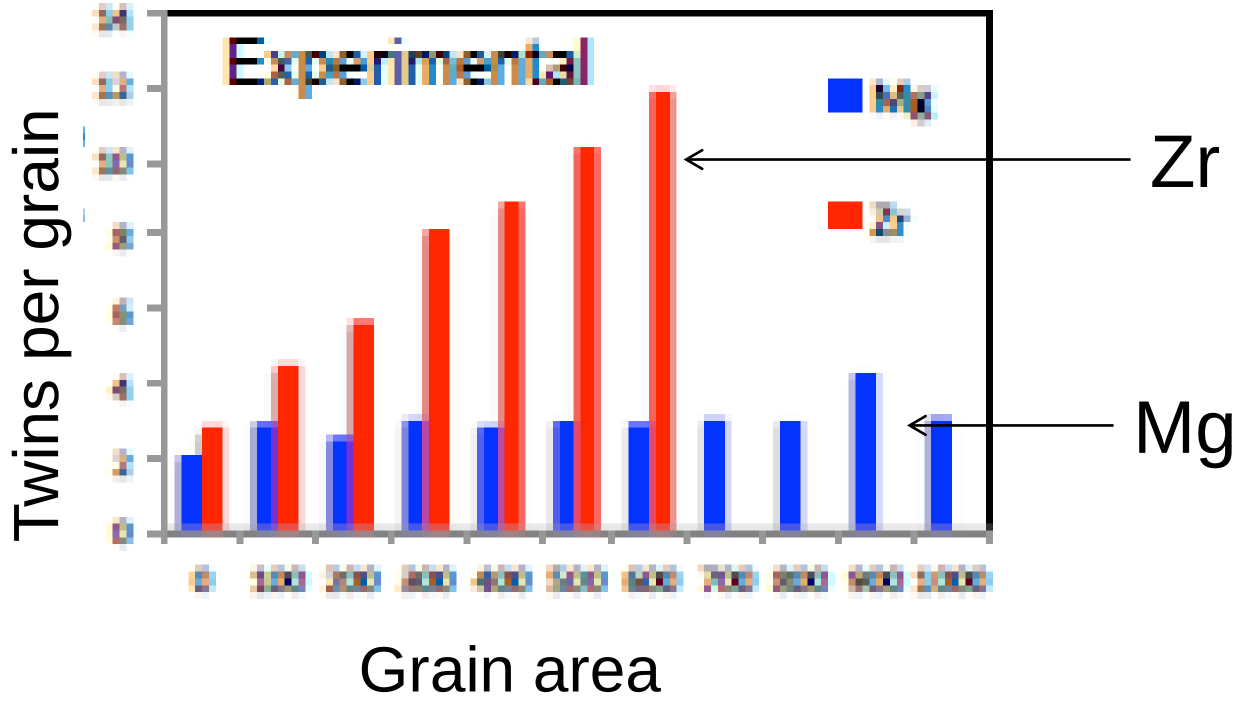
Situations where experiments cannot accurately characterize stress

- Effect of neighboring grain on twin local stresses
- Effect of twin-induced stresses on:
  - Twin transmission across grain boundaries
  - Twin growth
  - Twin separation

M. Arul Kumar, I.J. Beyerlein, C.N. Tomé
"Effect of local stress fields on twin characteristics in HCP metals"
Acta Materialia 116 (2016) 143-154

Effect of twin local stress on twin spacing

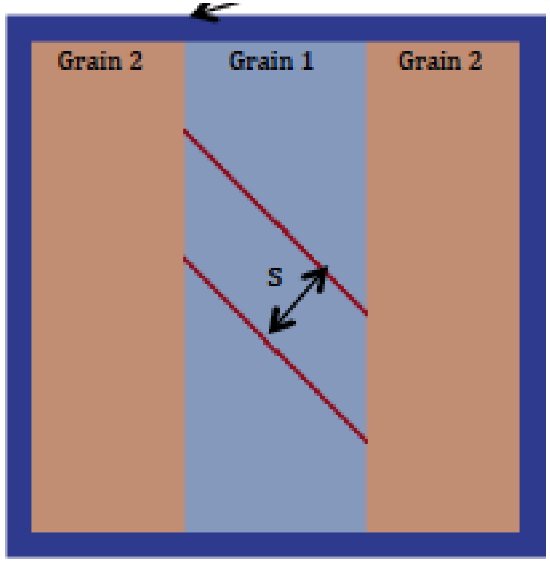
Number of twins per grain in Mg (3% IPC) and Zr (10% IPC)



EBSD statistics show thinner twins in Zr than in Mg
but closer to each other

Beyerlein et al, JMultCompEng (2011)

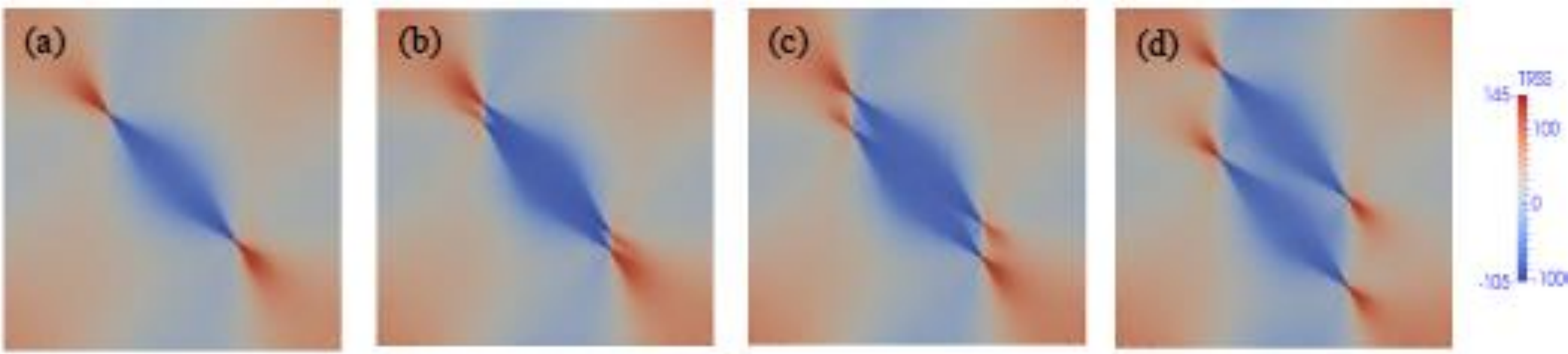
Effect of twin local stress on twin spacing



s : twin spacing
t : twin thickness

Material: Zr

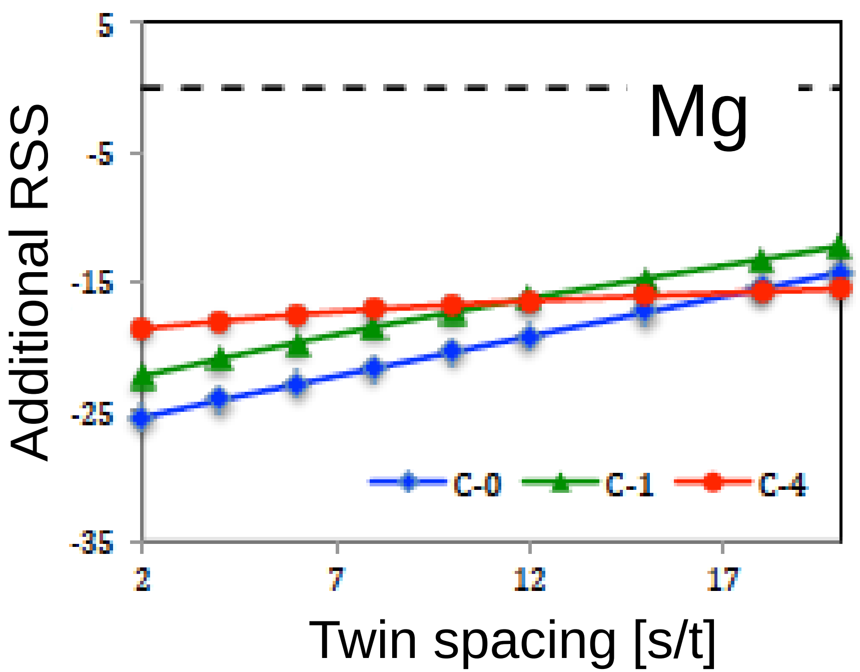
s = 0 (Single twin)　　s = 2t　　s = 8t　　s = 20t

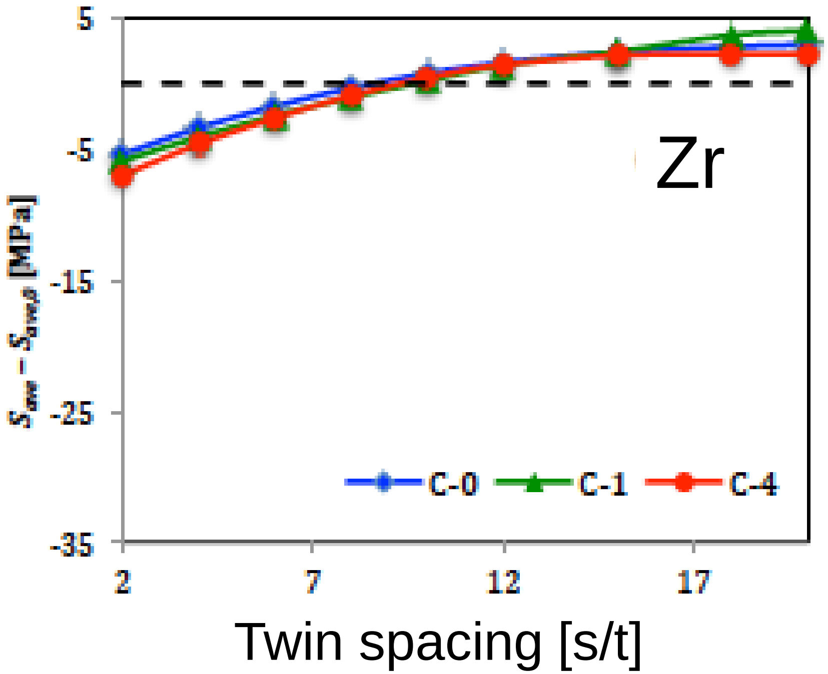


For parallel twins the coupling of the local twin fields decreases with increasing separation

Effect of twin local stress on twin spacing

Additional RSS on twin due to presence of another twin, as a function of separation





- Interaction between parallel twins is stronger in Mg than in Zr → as a consequence the minimum spacing between twins is larger in Mg than in Zr

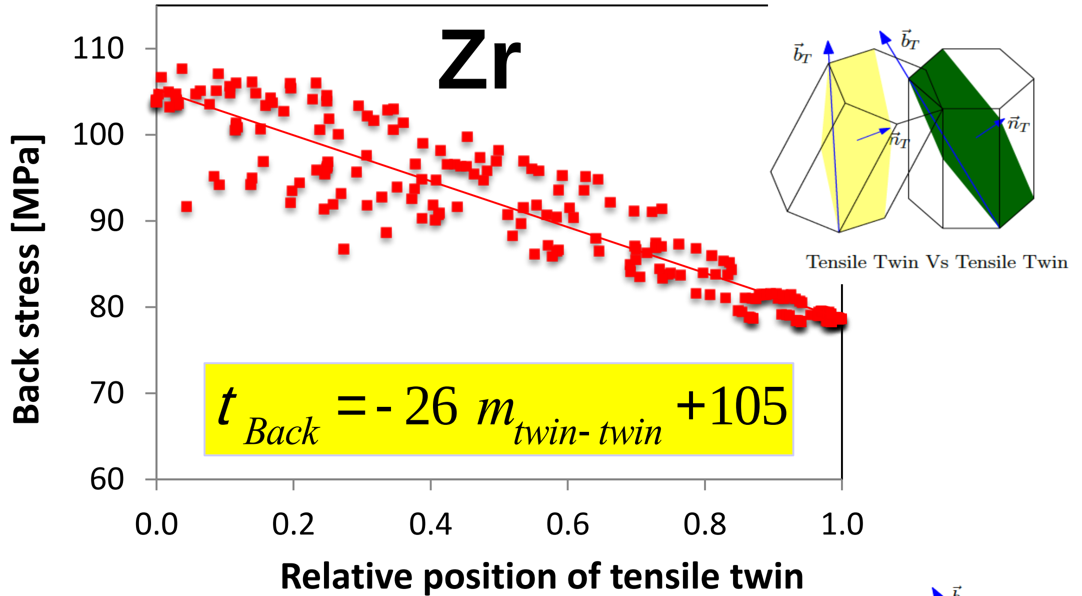
Summary

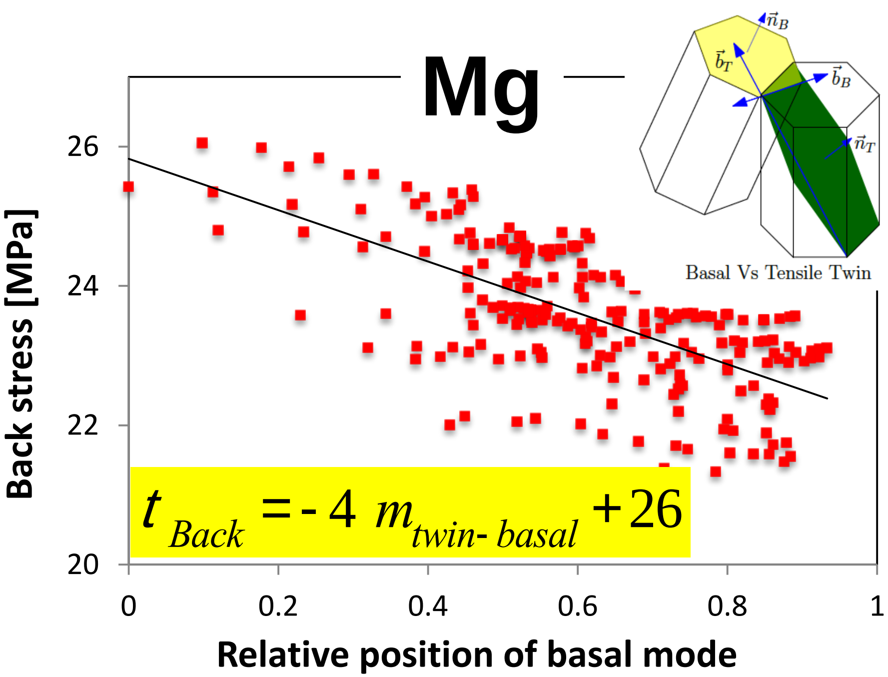
- Local stresses associated with twinning are highly heterogeneous
- Neighboring grain orientation has strong effect on twin back stress
- Plastic anisotropy plays a significant role on twinning processes
  - Twin growth is favorable in less anisotropic materials (eg., Mg)
  - Twin transmission and accommodation of multiple twins in a grain is favored in more plastically anisotropic materials (eg., Zr)

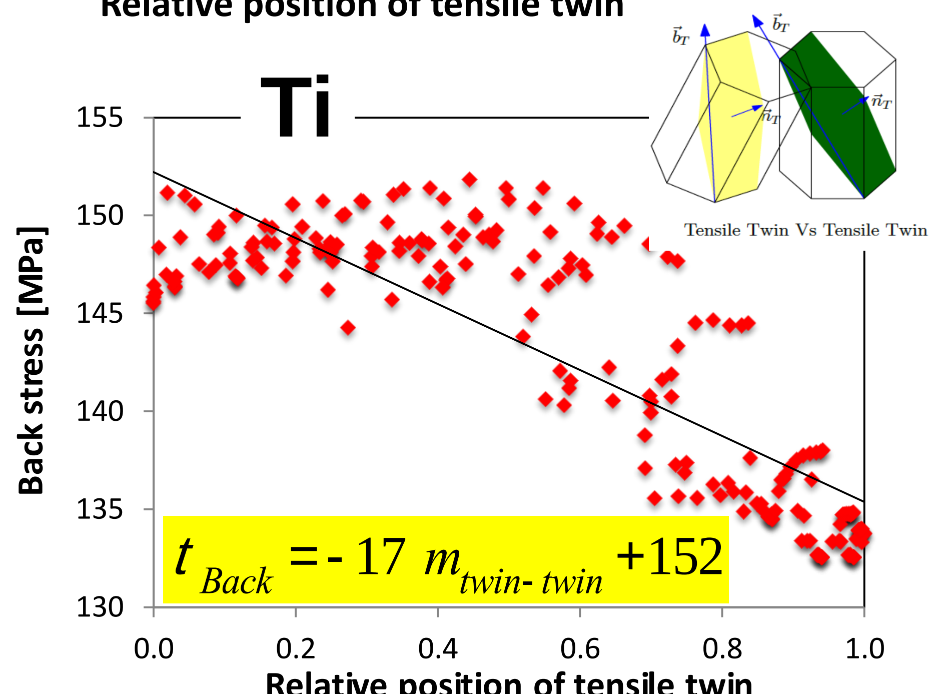
Results from local (micrometer scale) simulations are qualitatively in agreement with a wealth of statistical information on twins obtained from EBSD

Back stress as a function of neighbor misorientation

Deformation modes	CRSS values in MPa		
	Mg	Zr	Ti
Basal	3.3	700	120
Prism	36	20	60
Pyramidal	86	160	180
Tensile twin	20	102	125







Effect of material anisotropy on twin characteristics

Material	Elastic constants (GPa)					CRSS values of slip modes (MPa)			
	C11	C12	C13	C33	C44	Basal <a>	Prismatic <a>	Pyramidal <c+a>	T. Twin
Mg	59.75	23.24	21.70	61.70	16.39	3.3	35.7	86.2	20.0
Zr	143.5	72.50	65.40	164.9	32.10	700.0	20.0	160.0	102.0

Material	Elastic anisotropic indices		
Mg	0.98	1.11	1.21
Zr	0.78	1.11	1.47

Elastically and plastically Zr is more anisotropic than Mg !

Material	Twin characteristics		
	Twin growth	Number of twins per grain	Twin transmission
Less anisotropic Mg	Favorable	Only a few	Less favorable
More anisotropic Zr	Less favorable	more	Favorable